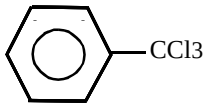
BENZOTRICHLORIDE

Benzotrichloride is a federal hazardous air pollutant and was identified as a toxic air contaminant in April 1993 under AB 2728.

CAS Registry Number: 98-07-7

Molecular Formula: $C_7H_5Cl_3$



Benzotrichloride is a clear, colorless to yellowish, oily liquid with a penetrating odor. It hydrolyzes in the presence of moisture forming benzoic and hydrochloric acids and it fumes in the air. Benzotrichloride is soluble in alcohol, ether, benzene, diethyl ether, ethanol, and many other organic solvents. It is insoluble in water (Merck, 1989).

Physical Properties of Benzotrichloride

Synonyms:	toluene trichloride; benzenyl trichloride; benzoic trichloride; phenyl chloroform; benzenyl chloride; benzylidyne chloride; phenyltrichloromethane; trichlorphenyl-methane; trichloromethyl-benzene
Molecular Weight:	195.48
Boiling Point:	220.8 °C
Melting Point:	-5 °C
Vapor Density:	6.77 (air = 1)
Vapor Pressure:	1 mm Hg at 45.8 °C
Density/Specific Gravity:	1.3759 at 20/4 °C (water = 1)
Log Octanol/Water Partition Coefficient:	2.92
Conversion Factor:	1 ppm = 7.99 mg/m^3

(HSDB, 1991; Merck, 1989; Sax, 1987; Sax, 1989; U.S. EPA, 1994a)

SOURCES AND EMISSIONS

A. Sources

Benzotrichloride is used as a chemical intermediate in the manufacture of benzoyl chloride, as a dye intermediate, and in organic syntheses (HSDB, 1991).

B. Emissions

No emissions of benzotrichloride from stationary sources in California were reported, based on data obtained from the Air Toxics "Hot Spots" Program (AB 2588) (ARB, 1997b).

C. Natural Occurrence

Benzotrichloride has not been reported to occur in nature (HSDB, 1991).

AMBIENT CONCENTRATIONS

No Air Resources Board data exist for ambient measurements of benzotrichloride.

INDOOR SOURCES AND CONCENTRATIONS

No information about the indoor sources and concentrations of benzotrichloride was found in the readily-available literature.

ATMOSPHERIC PERSISTENCE

No information about the atmospheric persistence of benzotrichloride was found in the readily-available literature.

AB 2588 RISK ASSESSMENT INFORMATION

Benzotrichloride emissions are not reported from stationary sources in California under the AB 2588 program. It is also not listed in the California Air Pollution Control Officers Association Air Toxics "Hot Spots" Program Revised 1992 Risk Assessment Guidelines as having health values (cancer or non-cancer) for use in risk assessments (CAPCOA, 1993).

HEALTH EFFECTS

Probable routes of human exposure to benzotrichloride are inhalation and dermal contact.

Non-Cancer: Benzotrichloride is a severe eye, nose, throat, and skin irritant in humans. In animals, large doses have caused central nervous system depression. No information is available on the chronic effects of benzotrichloride in humans. Mice and rats chronically exposed by inhalation have developed proliferative lesions of the respiratory tract. Also, adverse effects on the lymph nodes, liver, spleen, and kidneys have been reported in mice (U.S. EPA, 1994a).

The United States Environmental Protection Agency (U.S. EPA) has not established a

Reference Concentration (RfC) or an oral Reference Dose (RfD) for benzotrichloride. No information is available on adverse reproductive or developmental effects of benzotrichloride in humans. Rats exposed to benzotrichloride by gavage, have been reported to exhibit reduced maternal and fetal weight gain, and skeletal anomalies (U.S. EPA, 1994a).

Cancer: The U.S. EPA considers the several epidemiological studies that examined occupational exposure to the benzoyl peroxide production process involving benzotrichloride to be inadequate. In female mice exposed to benzotrichloride by inhalation, oral, and dermal routes, increased incidences of tumors at multiple sites have been observed. In mice exposed to benzotrichloride by inhalation, tumors of the lung, skin, and lymphoid tissue have been observed (U.S. EPA, 1994a).

The U.S. EPA has classified benzotrichloride in Group B2: Probable human carcinogen with an oral unit risk estimate of 3.6×10^{-4} (microgram per liter)$^{-1}$. This means that, if an individual were to ingest water containing benzotrichloride at 0.0036 micrograms per liter over an entire lifetime, that person would theoretically have no more than a 1 in 1 million increased chance of developing cancer (U.S. EPA, 1994a). The International Agency for Research on Cancer has not classified benzotrichloride as to its potential carcinogenicity in humans (IARC, 1987a). The State of California has determined under Proposition 65 that benzotrichloride is a carcinogen (CCR, 1996).